Lecture 4: Theoretical Fundamentals of Dynamic Programming

Diana Borsa

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This Lecture

- Last lecture: MDP, DP, Value Iteration (VI), Policy Iteration (PI)
- ► This lecture:
 - Deepen the mathematical formalism behind the MDP framework.
 - Revisit the Bellman equations and introduce their corresponding operators.
 - Re-visit the paradigm of dynamic programming: VI and PI.
- Next lectures: approximate, sampled versions of these paradigms, mainly in the absence of perfect knowledge of the environment.



Preliminaries

(Quick Recap of Functional Analysis)

Normed Vector Spaces

- Normed Vector Spaces: vector space \mathcal{X} + a norm $\|.\|$ on the elements of \mathcal{X} .
- Norms are defined a mapping $\mathcal{X} \to \mathbb{R}$ s.t:
 - 1. $||x|| \ge 0, \forall x \in \mathcal{X}$ and if ||x|| = 0 then $x = \mathbf{0}$.
 - 2. $\|\alpha x\| = |\alpha| \|x\|$ (homogeneity)
 - 3. $\|x_1 + x_2\| \le \|x_1\| + \|x_2\|$ (triangle inequality)
- For this lecture:
 - ightharpoonup Vector spaces: $\mathcal{X} = \mathbb{R}^d$
 - Norms:
 - ightharpoonup max-norm/ L_{∞} norm $\|.\|_{\infty}$
 - (weighted) L_2 norms $||.||_{2,\rho}$



Contraction Mapping

Definition

Let $\mathcal X$ be a vector space, equipped with a norm ||.||. An mapping $\mathcal T:\mathcal X\to\mathcal X$ is a α -contraction mapping if for any $x_1,x_2\in\mathcal X$, $\exists \alpha\in[0,1)$ s.t.

$$\|\mathcal{T}x_1 - \mathcal{T}x_2\| \le \alpha \|x_1 - x_2\|$$

- ▶ If $\alpha \in [0,1]$, then we call \mathcal{T} non-expanding
- Every contraction is also (by definition) Lipschitz, thus it is also continuous. In particular this means:

If
$$x_n \to_{\|.\|} x$$
 then $\mathcal{T}x_n \to_{\|.\|} \mathcal{T}x$



Fixed point

Definition

A point/vector $x \in \mathcal{X}$ is a fixed point of an operator \mathcal{T} if $\mathcal{T}x = x$.



Banach Fixed Point Theorem

Theorem (Banach Fixed Point Theorem)

Let $\mathcal X$ a complete normed vector space, equipped with a norm ||.|| and $\mathcal T:\mathcal X\to\mathcal X$ a γ -contraction mapping, then:

- 1. \mathcal{T} has a unique fixed point $x \in \mathcal{X}$: $\exists ! x^* \in \mathcal{X}$ s.t. $\mathcal{T}x^* = x^*$
- 2. $\forall x_0 \in \mathcal{X}$, the sequence $x_{n+1} = \mathcal{T}x_n$ converges to x^* in a geometric fashion:

$$||x_n - x^*|| \le \gamma^n ||x_0 - x^*||$$

Thus $\lim_{n\to\infty} ||x_n - x^*|| \le \lim_{n\to\infty} (\gamma^n ||x_0 - x^*||) = 0.$



Markov Decision Processes and Dynamic Programming

(Recap)



(Recap) MDPs

Markov Decision Processes (MDPs) formally describe an environment:

$$\mathcal{M} = (\mathcal{S}, \mathcal{A}, p, r, \gamma)$$

- ▶ Almost all RL problems can be formalised as MDPs, e.g.
 - Optimal control primarily deals with continuous MDPs
 - Partially observable problems can be converted into MDPs
 - Bandits are MDPs with one state



(Recap) Value functions

▶ State value function, for a policy π :

$$v_{\pi}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R_{t+1} | s_0 = s; \pi
ight]$$

Action value function, for a policy π :

$$q_{\pi}(s,a) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R_{t+1} | s_0 = s; a_0 = a, \pi
ight]$$

 $lackbox{ Optimal value functions: } q^* = \max_{\pi} q_{\pi} \ ig(v^* = \max_{\pi} v_{\pi} ig)$



(Recap) Bellman Equations

Theorem (Bellman Expectation Equations)

Given an MDP, $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$, for any policy π , the value functions obey the following expectation equations:

$$v_{\pi}(s) = \sum_{a} \pi(s, a) \left[r(s, a) + \gamma \sum_{s'} p(s'|a, s) v_{\pi}(s') \right]$$
 (1)

$$q_{\pi}(s,a) = r(s,a) + \gamma \sum_{s'} p(s'|a,s) \sum_{a' \in A} \pi(a'|s') q_{\pi}(s',a')$$
 (2)



(Recap) The Bellman Optimality Equation

Theorem (Bellman Optimality Equations)

Given an MDP, $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$, the optimal value functions obey the following expectation equations:

$$v^*(s) = \max_{a} \left[r(s, a) + \gamma \sum_{s'} p(s'|a, s) v^*(s') \right]$$
 (3)

$$q^*(s,a) = r(s,a) + \gamma \sum_{s'} p(s'|a,s) \max_{a' \in A} q^*(s',a')$$
 (4)



Bellman Operators



The Bellman Optimality Operator

Definition (Bellman Optimality Operator $T_{\mathcal{V}}^*$)

Given an MDP, $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$, let $\mathcal{V} \equiv \mathcal{V}_{\mathcal{S}}$ be the space of bounded real-valued functions over \mathcal{S} . We define, point-wise, the Bellman Optimality operator $T_{\mathcal{V}}^* : \mathcal{V} \to \mathcal{V}$ as:

$$(T_{\mathcal{V}}^*f)(s) = \max_{a} \left[r(s,a) + \gamma \sum_{s'} p(s'|a,s)f(s') \right], \ \forall f \in \mathcal{V}$$
 (5)

As a common convention we drop the index ${\mathcal V}$ and simply use ${\mathcal T}^*={\mathcal T}^*_{{\mathcal V}}$



Properties of the Bellman Operator T^*

1. It has one unique fixed point v^* .

$$T^*v^*=v^*$$

2. T^* is a γ -contraction wrt. to $\|.\|_{\infty}$

$$||T^*v - T^*u||_{\infty} \le \gamma ||v - u||_{\infty}, \forall u, v \in \mathcal{V}$$

3. T^* is monotonic:

$$\forall u, v \in \mathcal{V}$$
 s.t. $u \leq v$, component-wise, then $T^*u \leq T^*v$



Properties of the Bellman Operator T^* (Proofs)

Prop. (2): T^* is a γ -contraction wrt. to $\|.\|_{\infty}$

Proof

$$|T^*v(s) - T^*u(s)| = |\max_{a} [r(s, a) + \gamma \mathbb{E}_{s'|s, a} v(s')] - \max_{b} [r(s, b) + \gamma \mathbb{E}_{s''|s, b} u(s'')]| (6)$$

$$\leq \max_{a} |[r(s, a) + \gamma \mathbb{E}_{s'|s, a} v(s')] - [r(s, a) + \gamma \mathbb{E}_{s'|s, a} u(s')]| (7)$$

$$= \gamma \max_{a} |\mathbb{E}_{s'|s, a} [v(s') - u(s')]| (8)$$

$$\leq \gamma \max_{s'} |[v(s') - u(s')]| (9)$$

Thus we get:

$$||T^*v - T^*u||_{\infty} \le \gamma ||v - u||_{\infty}, \forall u, v \in \mathcal{V}$$

Note: Step (6)-(7) uses: $|\max_a f(a) - \max_b g(b)| \le \max_a |f(a) - g(a)|$



Properties of the Bellman Operator T^* (Proofs)

Prop. (3): T^* is monotonic

Proof

Given
$$v(s) \leq u(s), \forall s \Rightarrow r(s,a) + \mathbb{E}_{s'|s,a}u(s') \leq r(s,a) + \mathbb{E}_{s'|s,a}v(s')$$
.

$$T^*v(s) - T^*u(s) = \max_{a} \left[r(s,a) + \gamma \mathbb{E}_{s'|s,a} v(s') \right] - \max_{b} \left[r(s,b) + \gamma \mathbb{E}_{s''|s,b} u(s'') \right]$$
(10)
$$\leq \max_{a} \left(\left[r(s,a) + \gamma \mathbb{E}_{s'|s,a} v(s') \right] - \left[r(s,a) + \gamma \mathbb{E}_{s'|s,a} u(s') \right] \right)$$
(11)
$$\leq 0, \forall s.$$
(12)

Thus
$$T^*v(s) \leq T^*u(s), \forall s \in \mathcal{S}$$
.



Value Iteration through the lens of the Bellman Operator

Value Iteration

- ► Start with v_0 .
- ▶ Update values: $v_{k+1} = T^*v_k$.

As
$$k \to \infty$$
, $v_k \to_{\|.\|_{\infty}} v^*$.

Proof: Direct application of the *Banach Fixed Point Theorem*.

$$\begin{split} \|v_k - v^*\|_\infty &= \quad \|T^*v_{k-1} - v^*\|_\infty \\ &= \quad \|T^*v_{k-1} - T^*v^*\|_\infty \quad \text{(fixed point prop.)} \\ &\leq \quad \gamma \|v_{k-1} - v^*\|_\infty \quad \text{(contraction prop.)} \\ &\leq \quad \gamma^k \|v_0 - v^*\|_\infty \quad \text{(iterative application)} \end{split}$$



The Bellman Expectation Operator

Definition (Bellman Expectation Operator)

Given an MDP, $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$, let $\mathcal{V} \equiv \mathcal{V}_{\mathcal{S}}$ be the space of bounded real-valued functions over \mathcal{S} . For any policy $\pi: \mathcal{S} \times \mathcal{A} \to [0,1]$, we define, point-wise, the Bellman Expectation operator $\mathcal{T}^{\pi}_{\mathcal{V}}: \mathcal{V} \to \mathcal{V}$ as:

$$(T_{\mathcal{V}}^{\pi}f)(s) = \sum_{a} \pi(s, a) \left[r(s, a) + \gamma \sum_{s'} p(s'|a, s) f(s') \right], \ \forall f \in \mathcal{V}$$
 (13)



Properties of the Bellman Operator T^{π}

1. It has one unique fixed point v_{π} .

$$T^{\pi}v_{\pi}=v_{\pi}$$

2. T^{π} is a γ -contraction wrt. to $\|.\|_{\infty}$

$$||T^{\pi}v - T^{\pi}u||_{\infty} \leq \gamma ||v - u||_{\infty}, \forall u, v \in \mathcal{V}$$

3. T^{π} is monotonic:

$$\forall u, v \in \mathcal{V}$$
 s.t. $u \leq v$, component-wise, then $T^{\pi}u \leq T^{\pi}v$



Properties of the Bellman Operator T^{π} (Proofs)

Prop. (2): T^{π} is a γ -contraction wrt. to $\|.\|_{\infty}$

Proof

$$T^{\pi}v(s) - T^{\pi}u(s) = \sum_{a} \pi(a|s) \left[r(s,a) + \gamma \mathbb{E}_{s'|s,a}v(s') - r(s,a) - \gamma \mathbb{E}_{s'|s,a}u(s') \right]$$

$$= \gamma \sum_{a} \pi(a|s) \mathbb{E}_{s'|s,a} \left[v(s') - u(s') \right]$$

$$\Rightarrow |T^{\pi}v(s) - T^{\pi}u(s)| \leq \gamma \max_{s'} |\left[v(s') - u(s') \right]|$$
(14)

Thus we get:

$$||T^{\pi}v - T^{\pi}u||_{\infty} \le \gamma ||v - u||_{\infty}, \forall u, v \in \mathcal{V}$$

Note: (14) gives us also Prop. (3), monotonicity of T^{π} .



Policy Evaluation

(Iterative) Policy Evaluation

- ightharpoonup Start with v_0 .
- ▶ Update values: $v_{k+1} = T^{\pi}v_k$.

As
$$k \to \infty$$
, $v_k \to_{\|.\|_{\infty}} v_{\pi}$.

Proof: Direct application of the *Banach Fixed Point Theorem*.



(Summary) Dynamic Programming with Bellman Operators

Value Iteration

- \triangleright Start with v_0 .
- ▶ Update values: $v_{k+1} = T^*v_k$.

Policy Iteration

- ▶ Start with π_0 .
- ► Iterate:
 - Policy Evaluation: v_{π_i}
 - (E.g. For instance, by iterating T^{π} : $v_k = T^{\pi_i} v_{k-1} \Rightarrow v_k \to v^{\pi_i}$ as $k \to \infty$)
 - Greedy Improvement: $\pi_{i+1} = \arg \max_a q_{\pi_i}(s, a)$



Similarly for $q^{\pi}: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ functions

Definition (Bellman Expectation Operator)

Given an MDP, $\mathcal{M}=\langle\mathcal{S},\mathcal{A},p,r,\gamma\rangle$, let $\mathcal{Q}\equiv\mathcal{Q}_{\mathcal{S},\mathcal{A}}$ be the space of bounded real-valued functions over $\mathcal{S}\times\mathcal{A}$. For any policy $\pi:\mathcal{S}\times\mathcal{A}\to[0,1]$, we define, point-wise, the Bellman Expectation operator $T_{\mathcal{Q}}^{\pi}:\mathcal{Q}\to\mathcal{Q}$ as:

$$(T_{\mathcal{Q}}^{\pi}f)(s,a) = r(s,a) + \gamma \sum_{s'} p(s'|a,s) \sum_{a' \in \mathcal{A}} \pi(a'|s') f(s',a')$$
 , $\forall f \in \mathcal{Q}$

- This operator has unique fixed point which corresponds to the action-value function q_{π} in our MDP \mathcal{M} .
- ▶ Same properties as T^{π} : γ -contraction and monotonicity.



Similarly for $q^*: \mathcal{S} imes \mathcal{A} o \mathbb{R}$ functions

Definition (Bellman Optimality Operator)

Given an MDP, $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$, let $\mathcal{Q} \equiv \mathcal{Q}_{\mathcal{S}, \mathcal{A}}$ be the space of bounded real-valued functions over $\mathcal{S} \times \mathcal{A}$. We define the Bellman Optimality operator $T_{\mathcal{O}}^* : \mathcal{Q} \to \mathcal{Q}$ as:

$$(T_{\mathcal{Q}}^*f)(s,a) = r(s,a) + \gamma \sum_{s'} p(s'|a,s) \max_{a' \in \mathcal{A}} f(s',a')$$
 , $\forall f \in \mathcal{Q}$

- This operator has unique fixed point which corresponds to the action-value function q^* in our MDP \mathcal{M} .
- ▶ Same properties as T^* : γ -contraction and monotonicity.



Approximate Dynamic Programming



Approximate DP

- ➤ So far, we have assume perfect knowledge of the MDP and perfect/exact representation of the value functions.
- Realistically, more often than not:
 - We won't know the underlying MDP (like in the next two lectures)
 - ► We won't be able to represent the value function exactly after each update (lectures to come)



Approximate DP

- Realistically, more often than not:
 - ▶ We won't know the underlying MDP.
 - \Rightarrow sampling/estimation error, as we don't have access to the true operators T^{π} (T^*)
 - We won't be able to represent the value function exactly after each update.
 - ⇒ approximation error, as we approximate the true value functions within a (parametric) class (e.g. linear functions, neural nets, etc).
- Descrive: Under the above conditions, come up with a policy π that is (close to) optimal.



(Reminder) Value Iteration

Value Iteration

- ightharpoonup Start with v_0 .
- ▶ Update values: $v_{k+1} = T^*v_k$.

As $k \to \infty$, $v_k \to_{\|.\|_{\infty}} v^*$.



Approximate Value Iteration

Approximate Value Iteration

- ightharpoonup Start with v_0 .
- ▶ Update values: $v_{k+1} = AT^*v_k$.

$$(v_{k+1} \approx T^* v_k)$$

Question: As $k \to \infty$, $v_k \to_{\|.\|_{\infty}} v^*$? X

Answer: In general, no.



ADP: Approximating the value function

- ightharpoonup Using a function approximator $v_{\theta}(s)$, with a parameter vector $\theta \in \mathbb{R}^m$
- ightharpoonup The estimated value function at iteration k is $v_k = v_{\theta_k}$
- lacktriangle Use dynamic programming to compute $v_{ heta_{k+1}}$ from $v_{ heta_k}$

$$T^*v_k(s) = \max_{s} \mathbb{E}\left[R_{t+1} + \gamma v_k(S_{t+1}) \mid S_t = s\right]$$

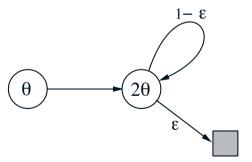
- Fit θ_{k+1} s.t. $v_{\theta_{k+1}} \approx T^* v_k(s)$
 - ▶ For instance, with respect to a squared loss over the state-space.

$$heta_{k+1} = rg \min_{ heta_{k+1}} \sum_s (v_{ heta_{k+1}}(s) - T^*v_k(s))^2$$



Example of divergence with dynamic programming

➤ Tsitsiklis and Van Roy made an example where dynamic programming with linear function approximation can diverge. Consider the two state example below, where the rewards are all zero, there are no decisions, and there is a single parameter for estimating the value.



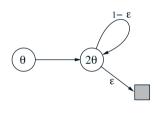


Blackboard

(Tsitsiklis and Van Roy's Example)

Example of divergence with dynamic programming

➤ Tsitsiklis and Van Roy made an example where dynamic programming with linear function approximation can diverge. Consider the two state example below, where the rewards are all zero, there are no decisions, and there is a single parameter for estimating the value.



$$\begin{aligned} \theta_{k+1} &= \underset{\theta}{\operatorname{argmin}} \ \sum_{s \in \mathcal{S}} (v_{\theta}(s) - \mathbb{E} \left[v_{\theta_k}(S_{t+1}) \mid S_t = s \right])^2 \\ &= \underset{\theta}{\operatorname{argmin}} \ (\theta - \gamma 2\theta_k)^2 + (2\theta - \gamma(1 - \epsilon)2\theta_k)^2 \\ &= \frac{2(3 - 2\epsilon)\gamma}{5} \theta_k \end{aligned}$$

- ▶ What is $\lim_{k\to\infty}\theta_k$ when $\theta_0=1$, $\epsilon=\frac{1}{8}$, and $\gamma=1$?
- ► This is only a problem when we update the states, e.g., synchronously, without looking at the time an agent would spend in each state



Approximate Value Iteration

Approximate Value Iteration

- ightharpoonup Start with v_0 .
- ▶ Update values: $v_{k+1} = AT^*v_k$.

 $(v_{k+1} \approx T^* v_k)$

Question: As $k \to \infty$, $v_k \to_{\|.\|_{\infty}} v^*$? X

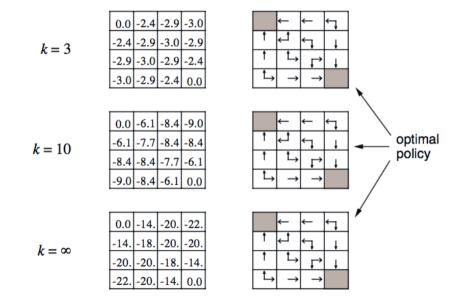
Answer: In general, no.

Hopeless? Not quite!

- ▶ Sample versions of these algorithms converge under mild conditions
- Even for the function approximation case, the theoretical danger of divergence is rarely materialised in practice
- There may many value functions that can induce the optimal policy!



Example from last lecture: Many value functions ⇒ same optimal policy



Performance of a Greedy Policy

Theorem (Value of greedy policy)

Consider a MDP. Let $q: S \times A \to \mathbb{R}$ be an arbitrary function and let π be the greedy policy associated with q, then:

$$\|q^*-q^\pi\|_\infty \leq rac{2\gamma}{1-\gamma}\|q^*-q\|_\infty$$

where q^* is the optimal value function associated with this MDP.



Performance of a Greedy Policy (Proof)

Statement:
$$\|q^*-q^\pi\|_\infty \leq rac{2\gamma}{1-\gamma}\|q^*-q\|_\infty$$

Re-arranging: $(1 - \gamma) \| a^* - a^{\pi} \|_{\infty} < 2\gamma \| a^* - a \|_{\infty}$.

Proof

$$\|q^{*} - q^{\pi}\|_{\infty} = \|q^{*} - T^{\pi}q + T^{\pi}q - q^{\pi}\|_{\infty}$$

$$\leq \|q^{*} - T^{\pi}q\|_{\infty} + \|T^{\pi}q - q^{\pi}\|_{\infty}$$

$$= \|T^{*}q^{*} - T^{*}q\|_{\infty} + \|T^{\pi}q - T^{\pi}q^{\pi}\|_{\infty}$$

$$\leq \gamma \|q^{*} - q\|_{\infty} + \gamma \underbrace{\|q - q^{\pi}\|_{\infty}}_{\leq \|q - q^{*}\|_{\infty} + \|q^{*} - q^{\pi}\|_{\infty}}$$

$$\leq 2\gamma \|q^{*} - q\|_{\infty} + \gamma \|q^{*} - q^{\pi}\|_{\infty}$$

$$\leq 2\gamma \|q^{*} - q\|_{\infty} + \gamma \|q^{*} - q^{\pi}\|_{\infty}$$

$$(15)$$

$$(16)$$

$$\leq ||q - q^{*}||_{\infty} + ||q^{*} - q^{*}||_{\infty}$$

$$\leq ||q - q^{*}||_{\infty} + ||q^{*} - q^{*}||_{\infty}$$

$$(19)$$



Performance of a Greedy Policy: Test your understanding!

Theorem (Value of greedy policy)

Consider a MDP. Let $q: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ be an arbitrary function and let π be the greedy policy associated with q, then:

$$\|q^*-q^\pi\|_\infty \leq rac{2\gamma}{1-\gamma}\|q^*-q\|_\infty$$

where q^* is the optimal value function associated with this MDP.

Observations:

- ightharpoonup Small values of γ obtain a better(smaller) upper bound on the potential loss of performance. How do you interpret that?
- ▶ In particular, what happens for $\gamma = 0$? How do you explain this?
- ▶ What if $q = q^*$? What does this bound imply in that case?



(Reminder) Policy Iteration

Policy Iteration

- ▶ Start with π_0 .
- ► Iterate:
 - Policy Evaluation: $q_i = q_{\pi_i}$
 - Greedy Improvement: $\pi_{i+1} = \arg \max_a q_{\pi_i}(s, a)$

As $i \to \infty$, $q_i \to_{\parallel,\parallel_{\infty}} q^*$. Thus $\pi_i \to \pi^*$.



Approximate Policy Iteration

Approximate Policy Iteration

- ▶ Start with π_0 .
- ► Iterate:
 - Policy Evaluation: $q_i = \mathcal{A}q_{\pi_i}$ $(q_i \approx q_{\pi_i})$
 - Greedy Improvement: $\pi_{i+1} = \arg \max_a \frac{q_i(s, a)}{q_i(s, a)}$

Question 1: As $i \to \infty$, does $q_i \to_{\|.\|_{\infty}} q^*$? X

Answer: In general, no.

Question 2: Or does π_i converge to the optimal policy? X

Answer: In general, no.

Hopeless? In some cases, no, depending on the nature of A. (More: Next lectures)



(Summary) Approximate Dynamic Programming

Approximate Value Iteration

- ightharpoonup Start with v_0 .
- ▶ Update values: $v_{k+1} = AT^*v_k$.

$(v_{k+1} \approx T^* v_k)$

Approximate Policy Iteration

- ightharpoonup Start with π_0 .
- Iterate:
 - Policy Evaluation: $q_i = Aq_{\pi_i}$
 - Greedy Improvement: $\pi_{i+1} = \arg \max_a \frac{q_i(s, a)}{q_i(s, a)}$

$$(q_i \approx q_{\pi_i})$$



Questions?

The only stupid question is the one you were afraid to ask but never did. -Rich Sutton

For questions that may arise during this lecture please use Moodle and/or the next Q&A session.

